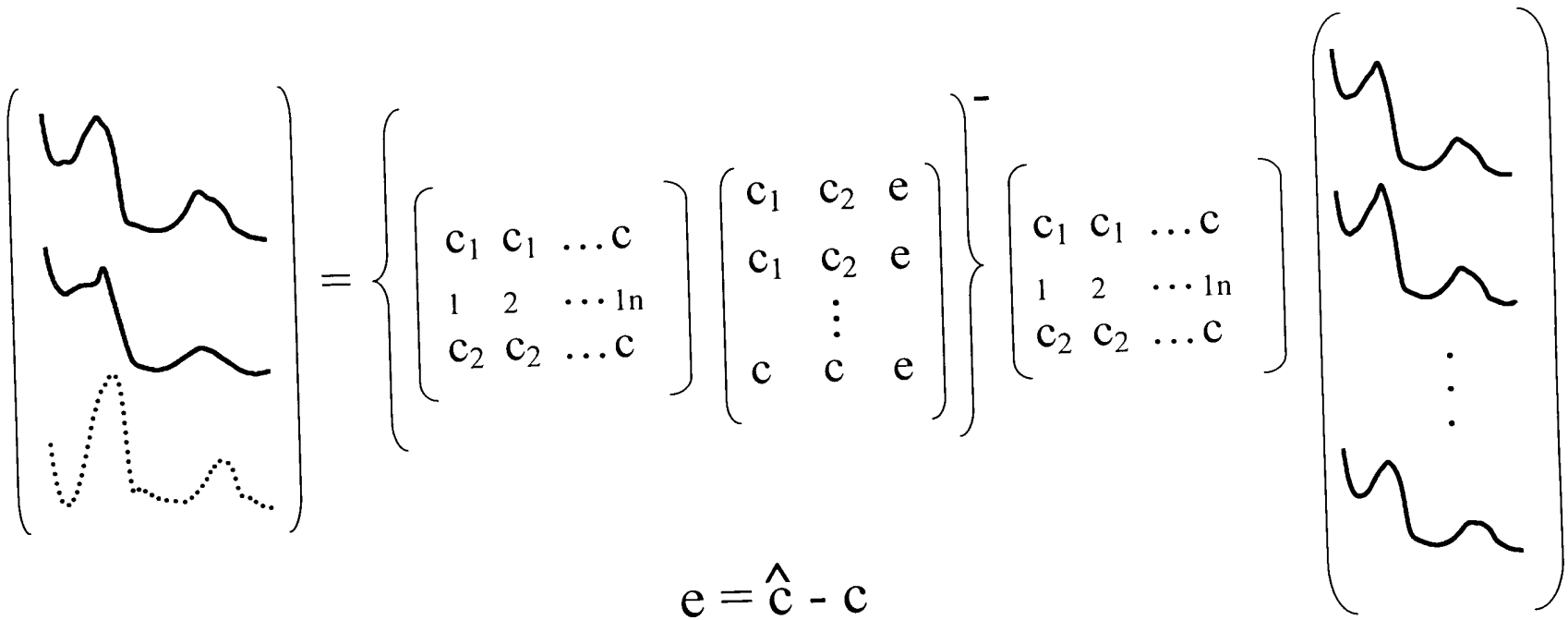
$$\hat{\tilde{K}} = ( \tilde{C}^T \tilde{C} )^{-1} \tilde{C}^T$$




$$e = \hat{c} - c$$

**Fig. 1**

$$\hat{\tilde{\tilde{C}}} = A \quad \hat{\tilde{\tilde{K}}}^T \quad (\hat{\tilde{\tilde{K}}} \quad \hat{\tilde{\tilde{K}}}^T)^{-1}$$

$$\begin{pmatrix} \hat{c}_1 & \hat{c}_2 & \hat{c}_e \\ \hat{c}_1 & \hat{c}_2 & \hat{c}_e \\ \vdots & & \\ \hat{c} & \hat{c} & \hat{c}_e \end{pmatrix} = \left( \begin{array}{c} \\ \\ \\ \vdots \\ \\ \\ \end{array} \right) \left\{ \left( \begin{array}{c} \\ \\ \\ \\ \\ \\ \end{array} \right) \left\{ \left( \begin{array}{c} \\ \\ \\ \\ \\ \\ \end{array} \right) \left( \begin{array}{c} \\ \\ \\ \\ \\ \\ \end{array} \right) \right\}^{-}$$

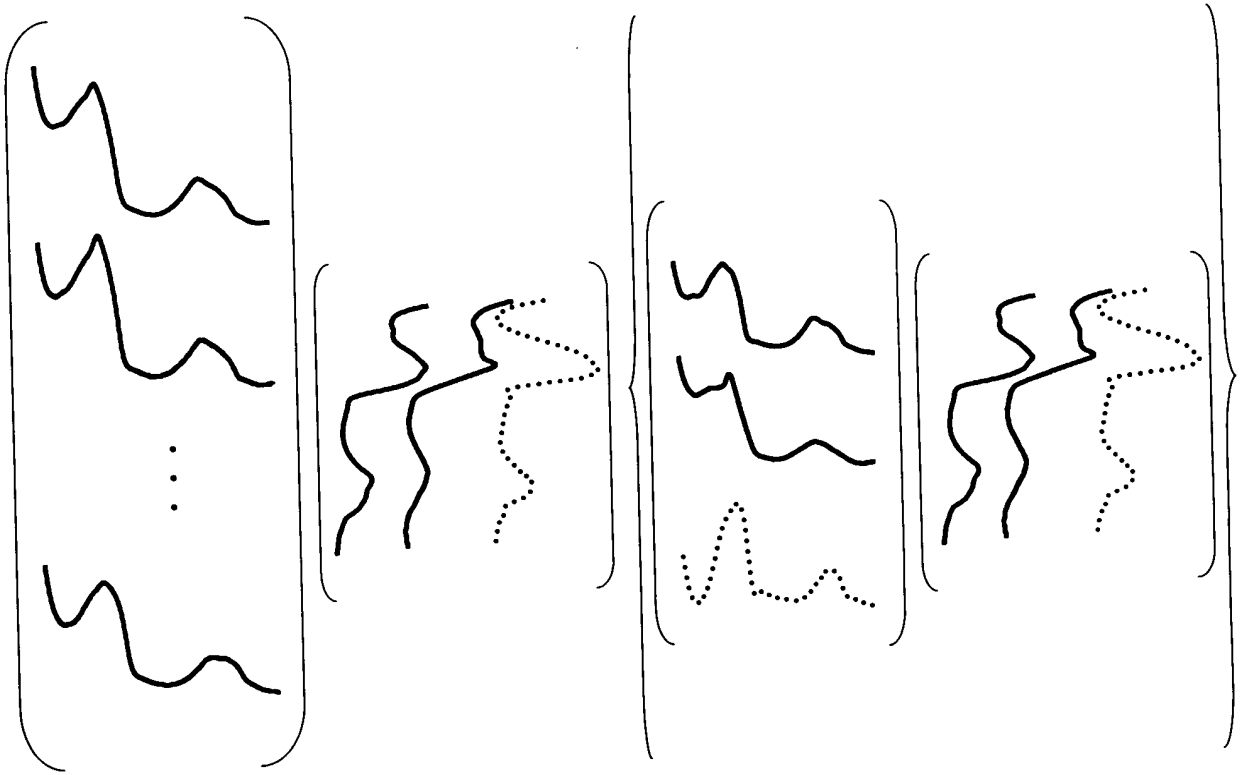


**Fig. 2**

# Spectral-Residual Augmented CLS

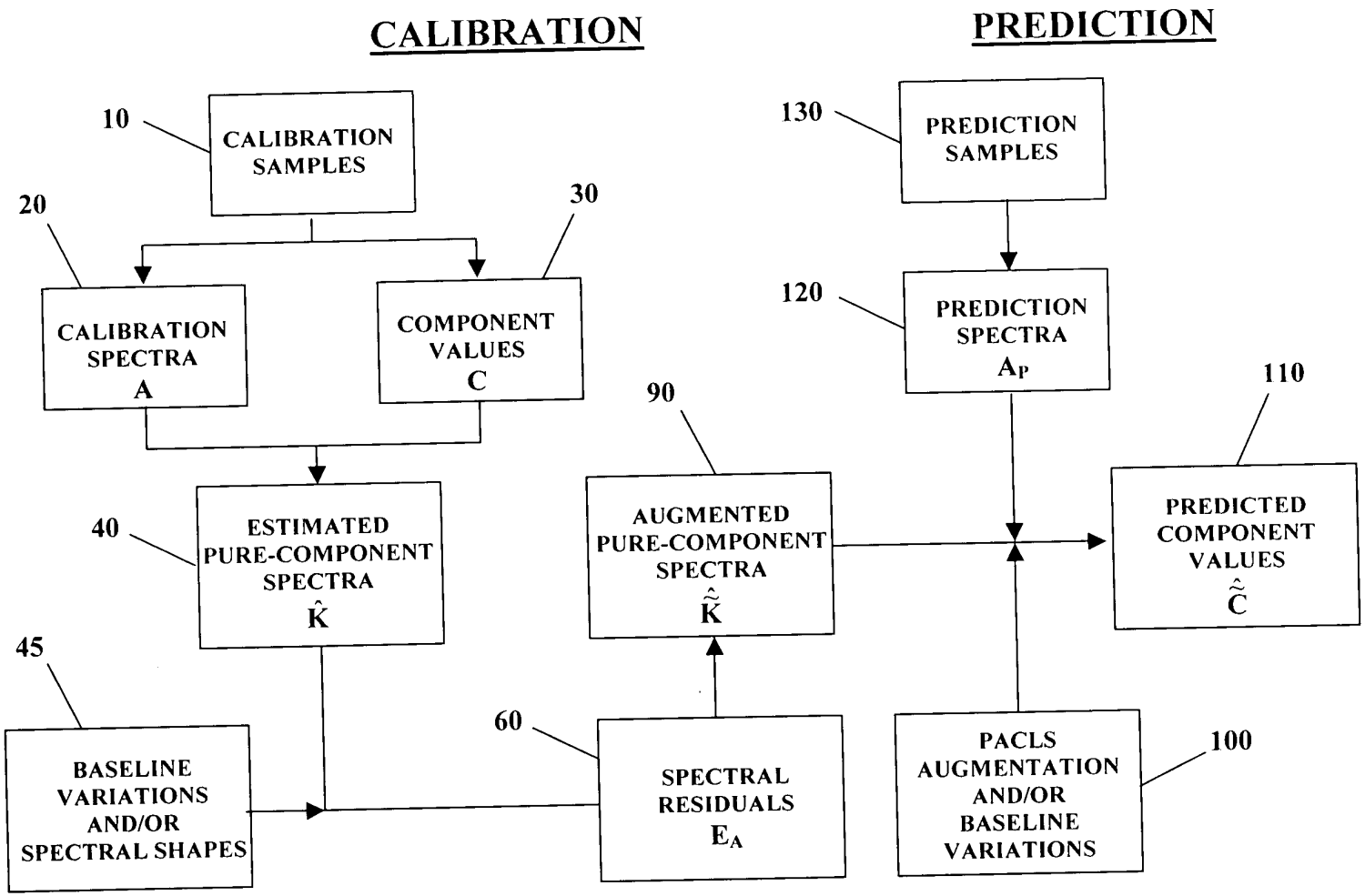



Fig. 3A

# Scores Augmented CLS

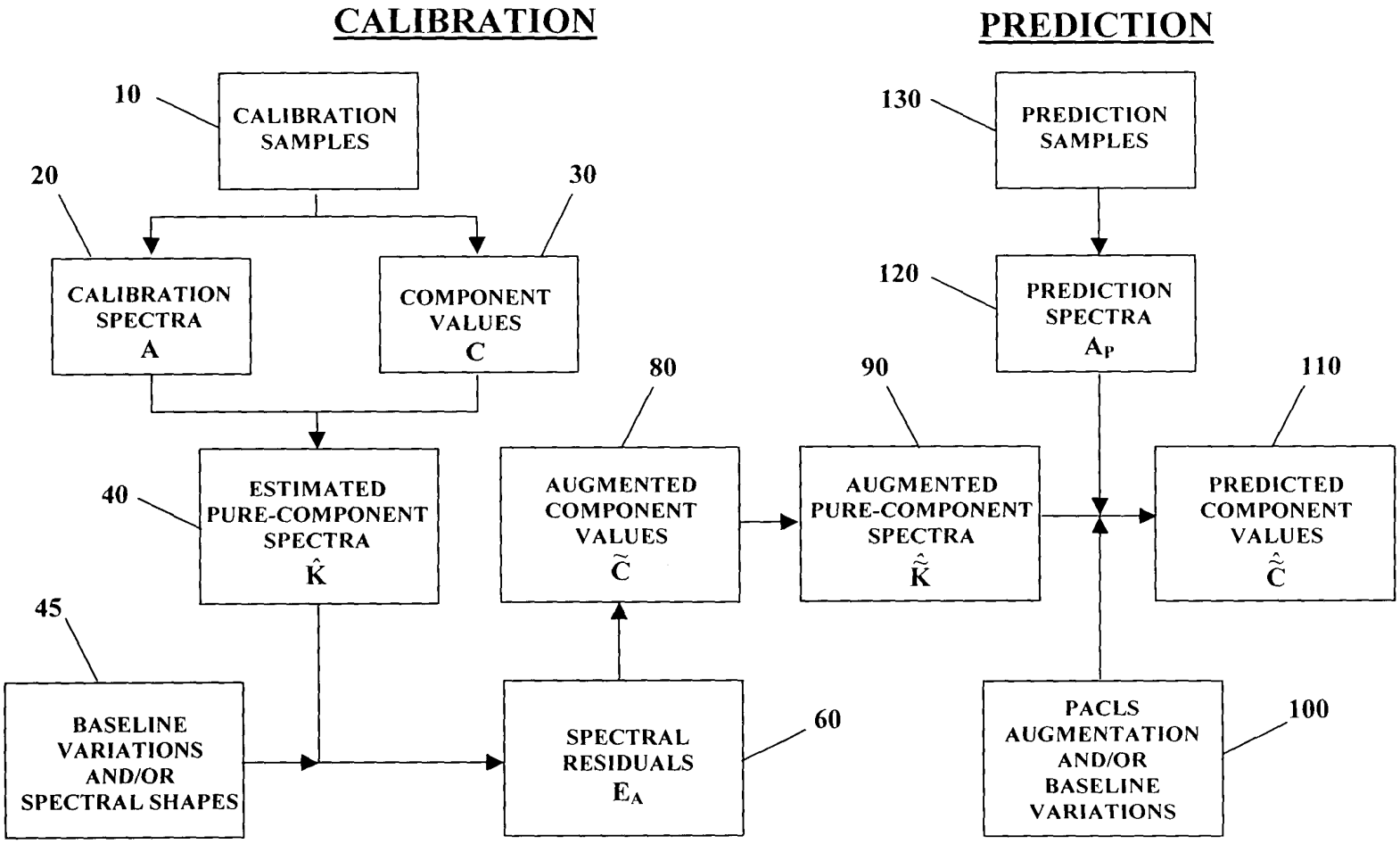



Fig. 3B

# Concentration-Residual Augmented CLS

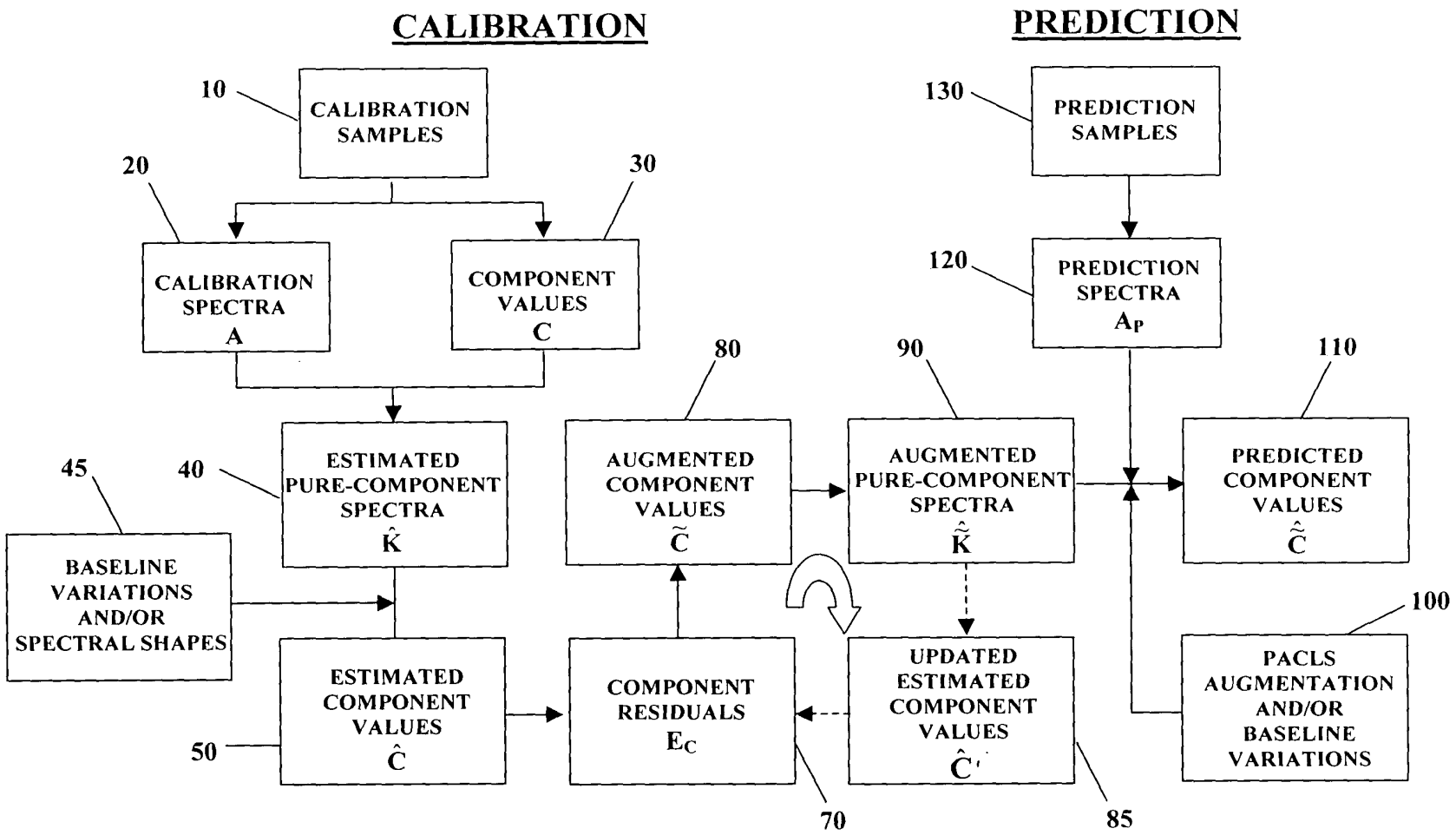



Fig. 4

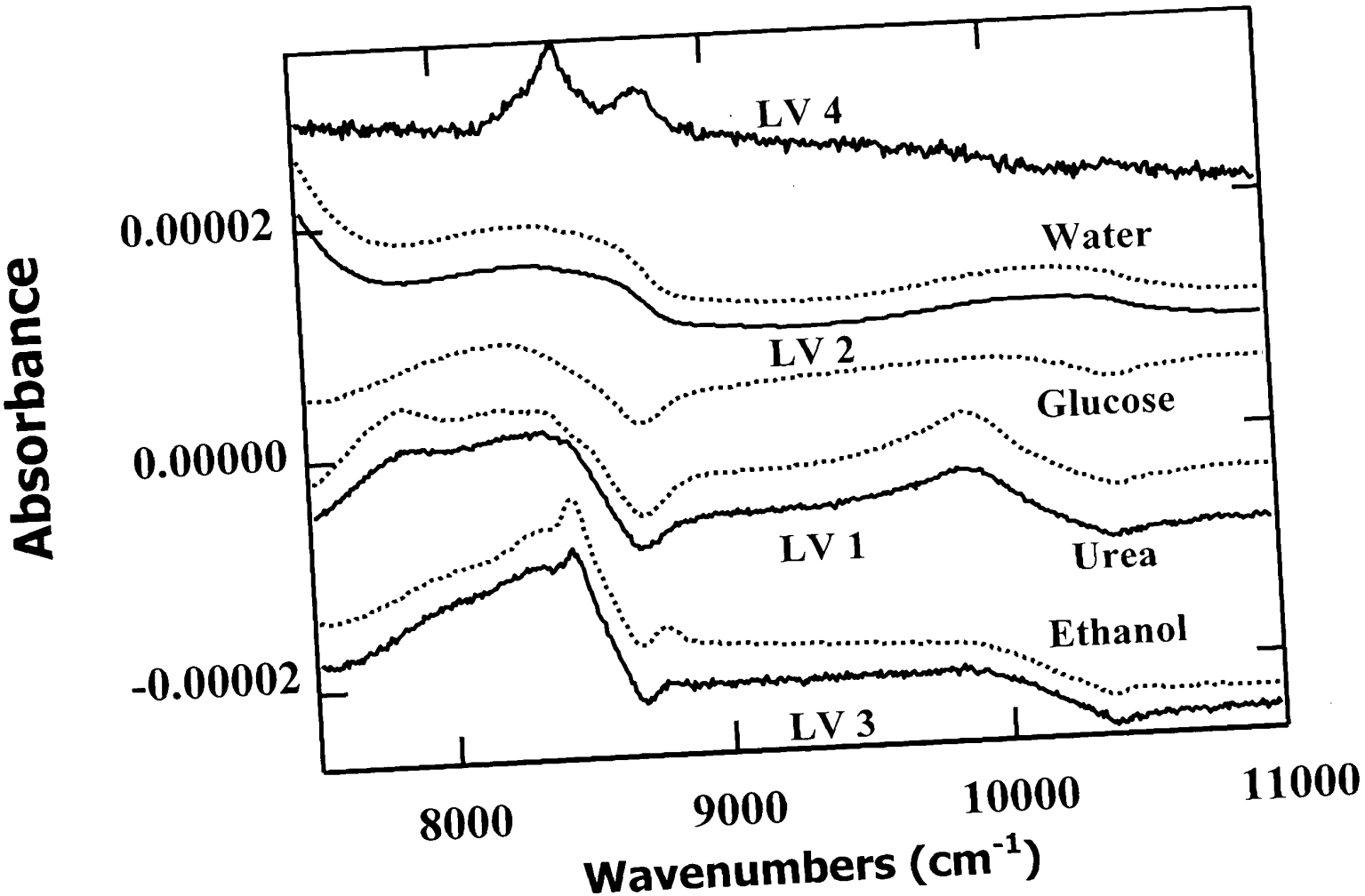

LV 4
Water
LV 2
Glucose
LV 1
Urea
Ethanol
LV 3
0.00002
0.00000
-0.00002
Absorbance
8000
9000
10000
11000
Wavenumbers (cm-1)

Fig. 5

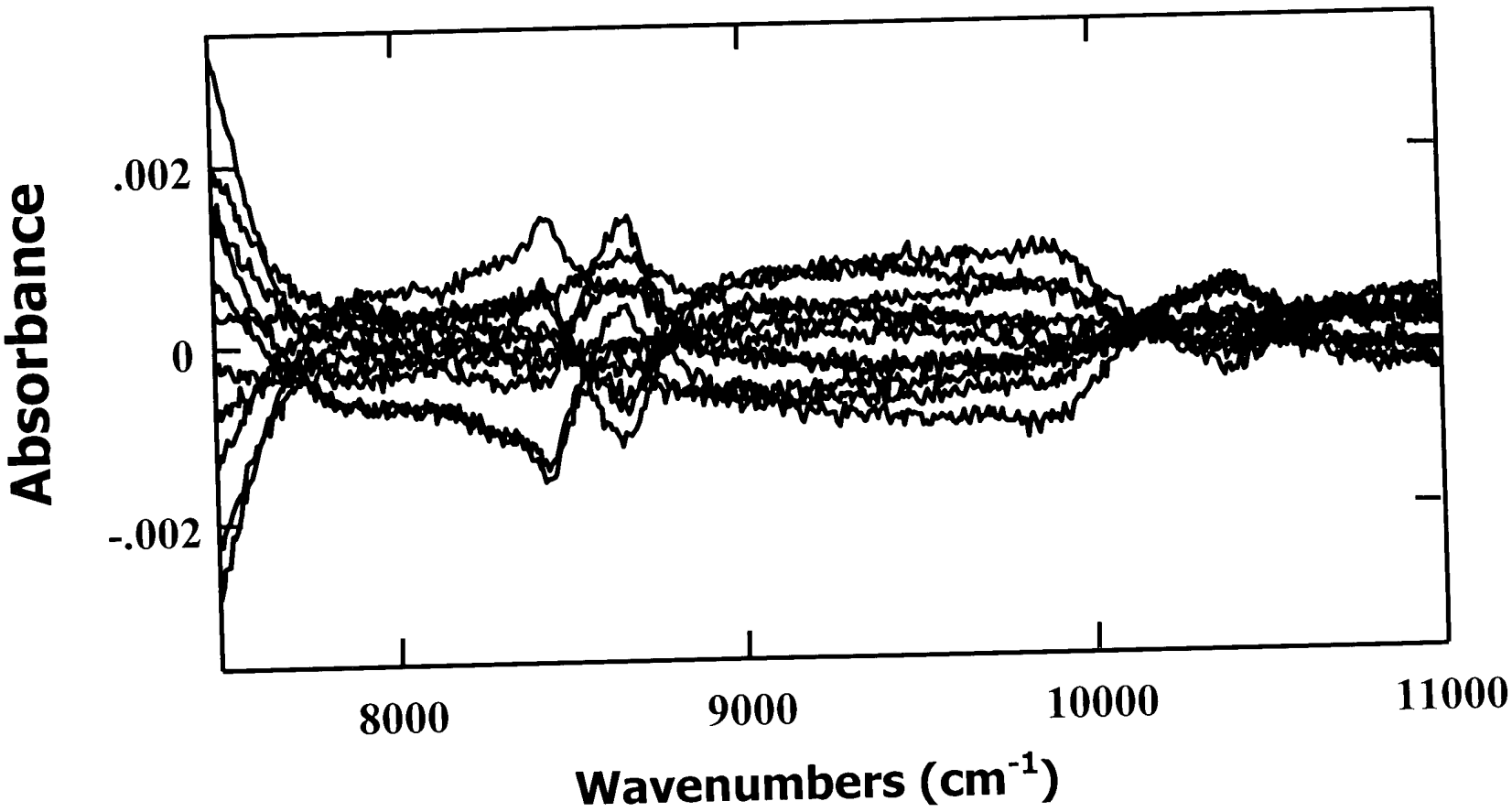



Fig. 6

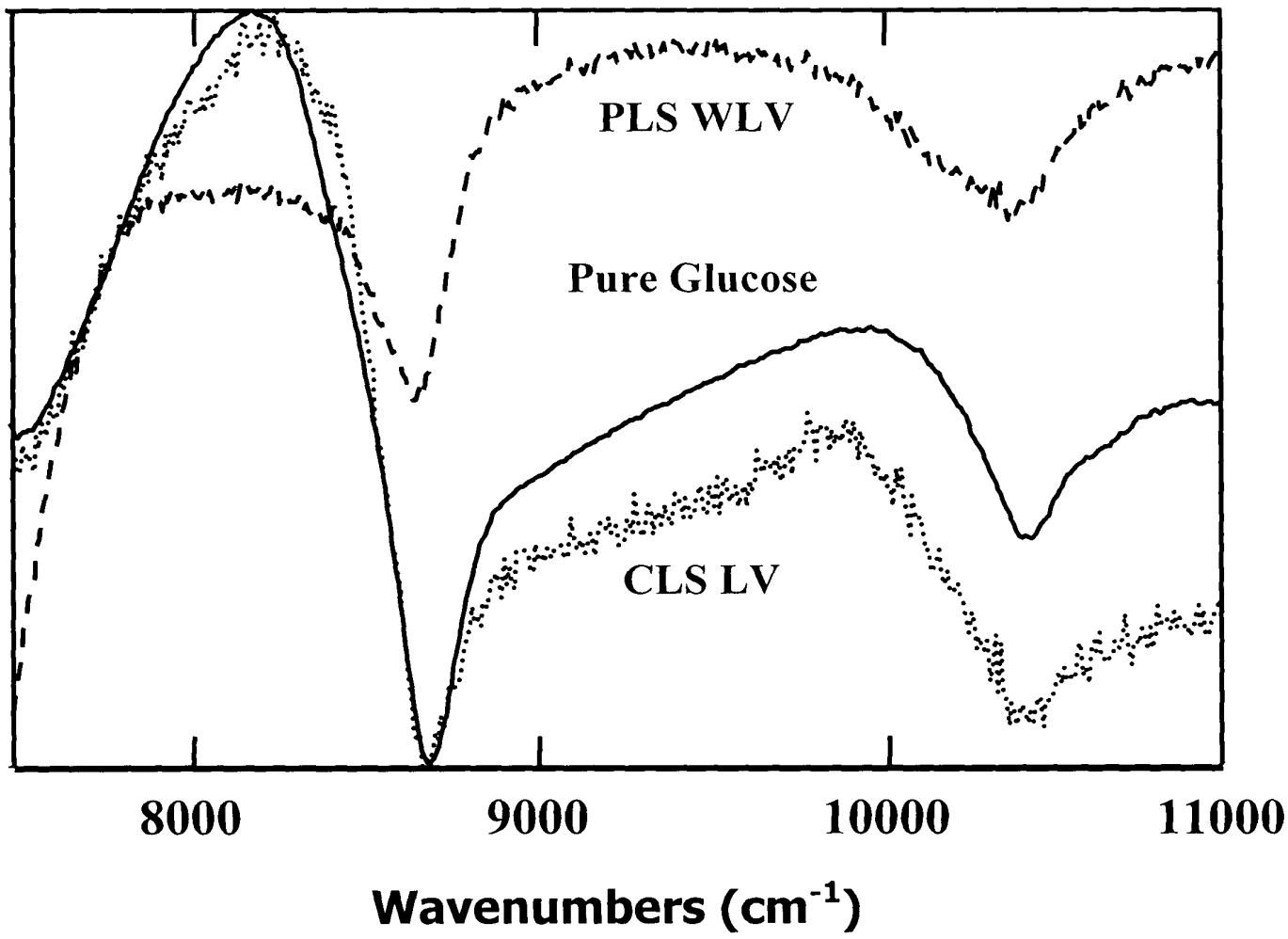

PLS WLV
Pure Glucose
CLS LV
8000
9000
10000
11000
Wavenumbers (cm-1)

Fig. 7

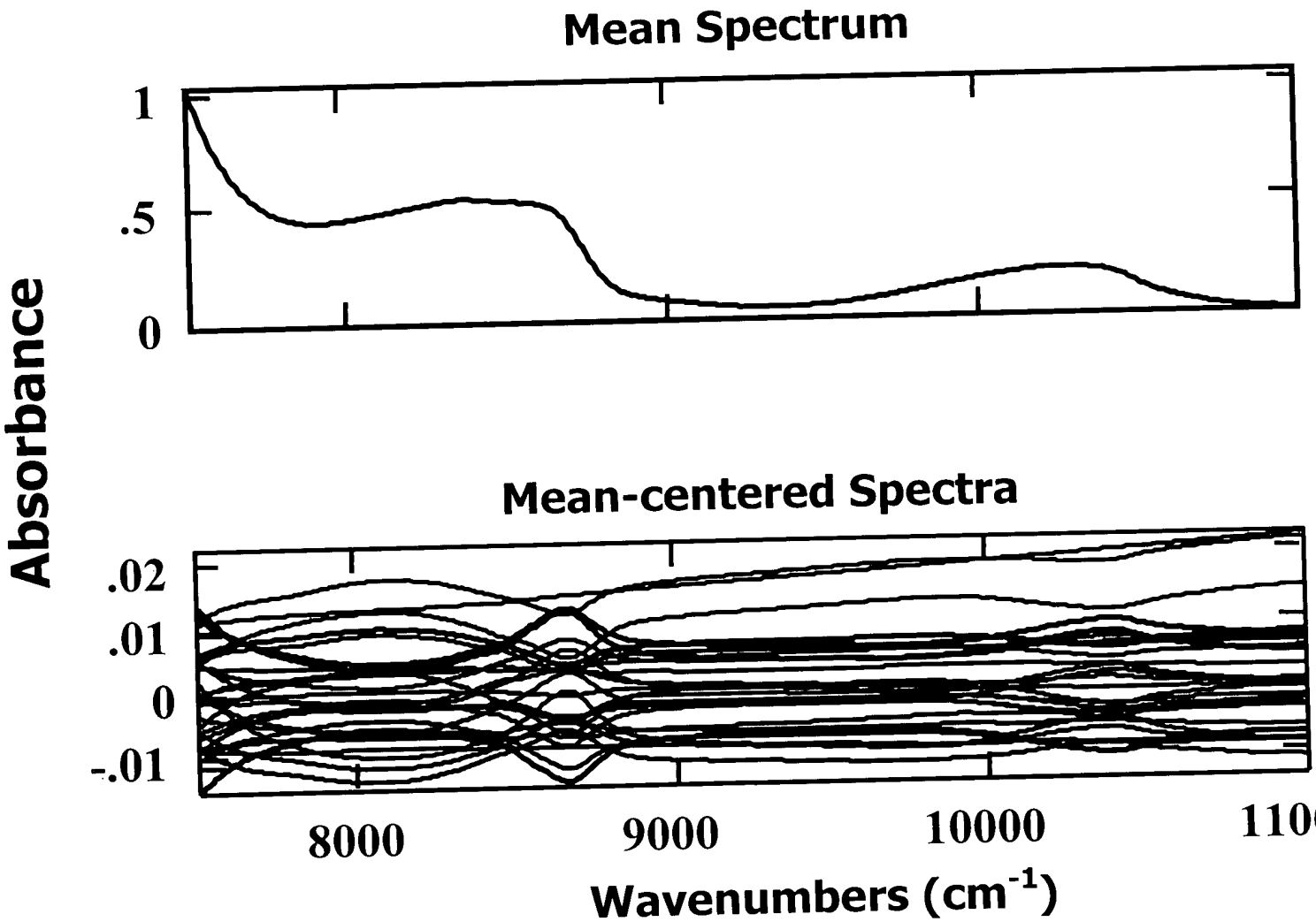

Mean Spectrum
1
.5
0
Absorbance
Mean-centered Spectra
.02
.01
0
-.01
8000
9000
10000
11000
Wavenumbers (cm-1)

Fig. 8A

Fig. 8B

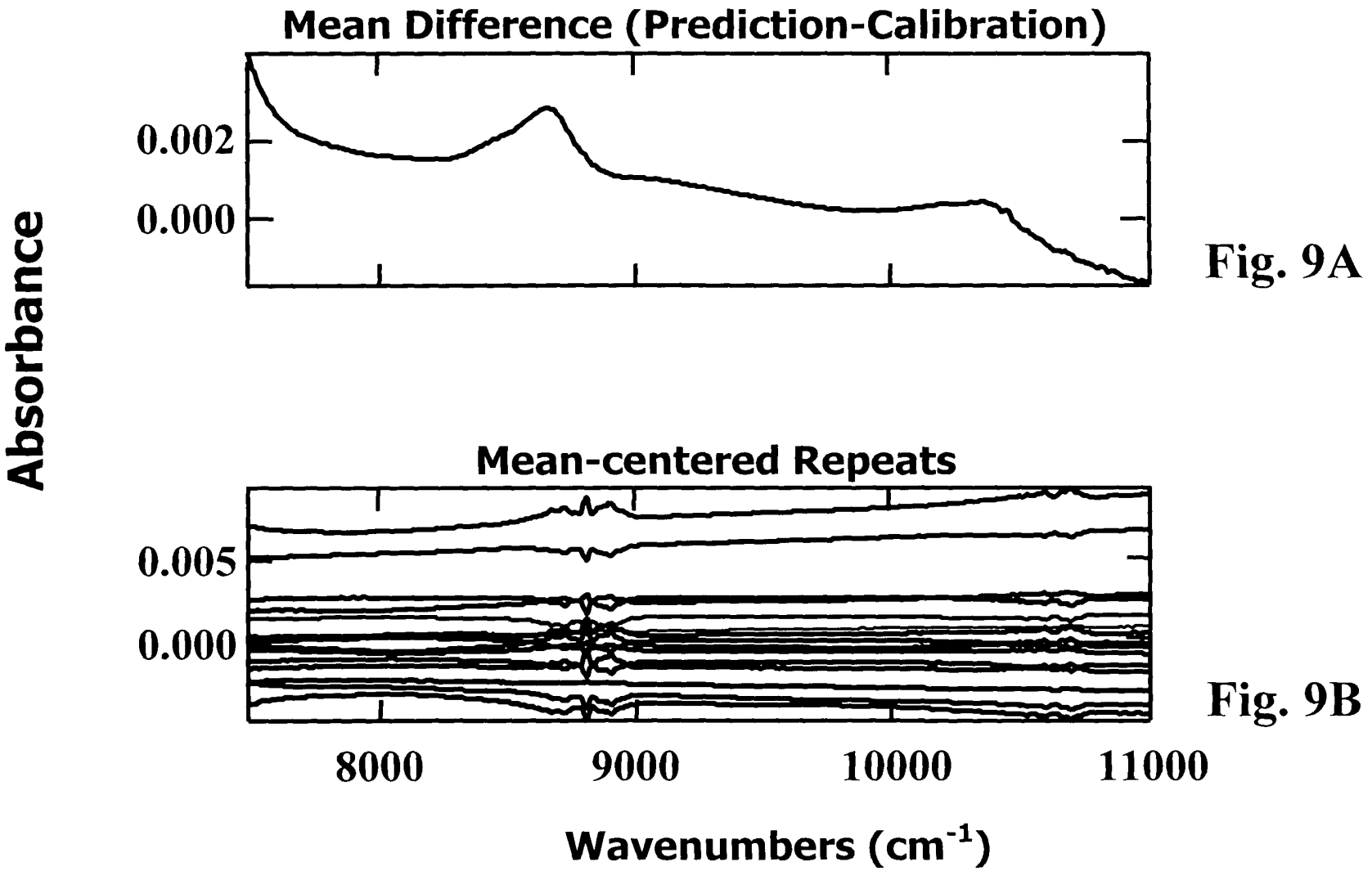

Mean Difference (Prediction-Calibration)
0.002
0.000
Absorbance
Mean-centered Repeats
0.005
0.000
8000
9000
10000
11000
Wavenumbers (cm-1)

Fig. 9A

Fig. 9B

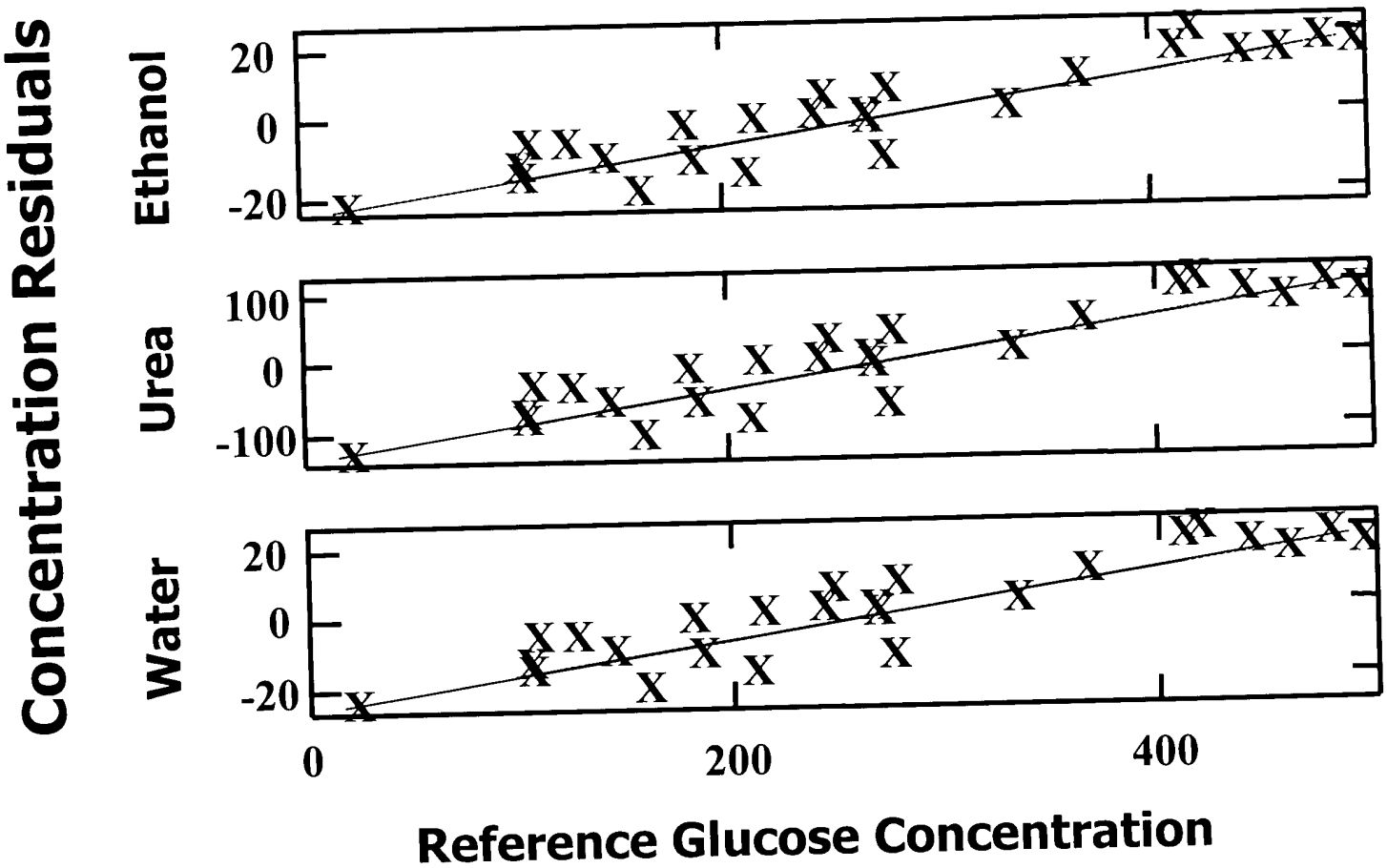



Fig. 10A

Fig. 10B

Fig. 10C

# Augmented Alternating CLS

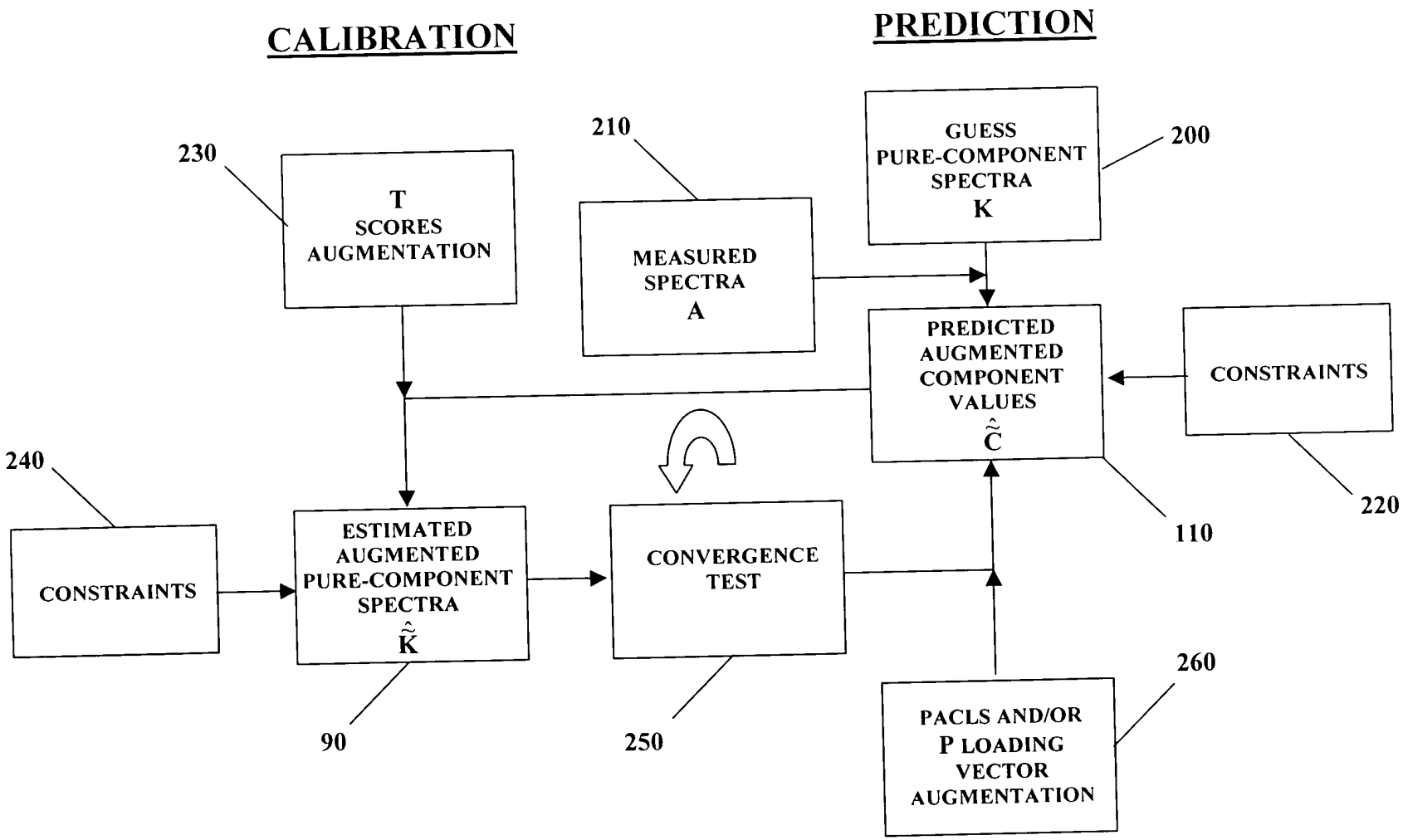



Fig. 11

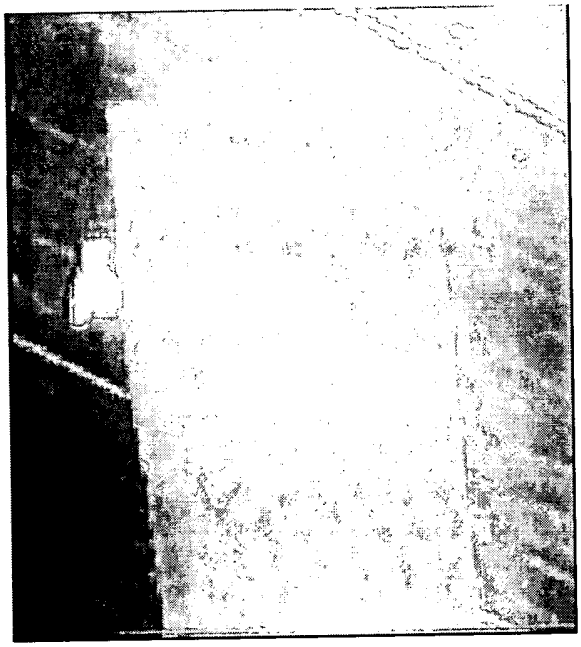


Fig. 12

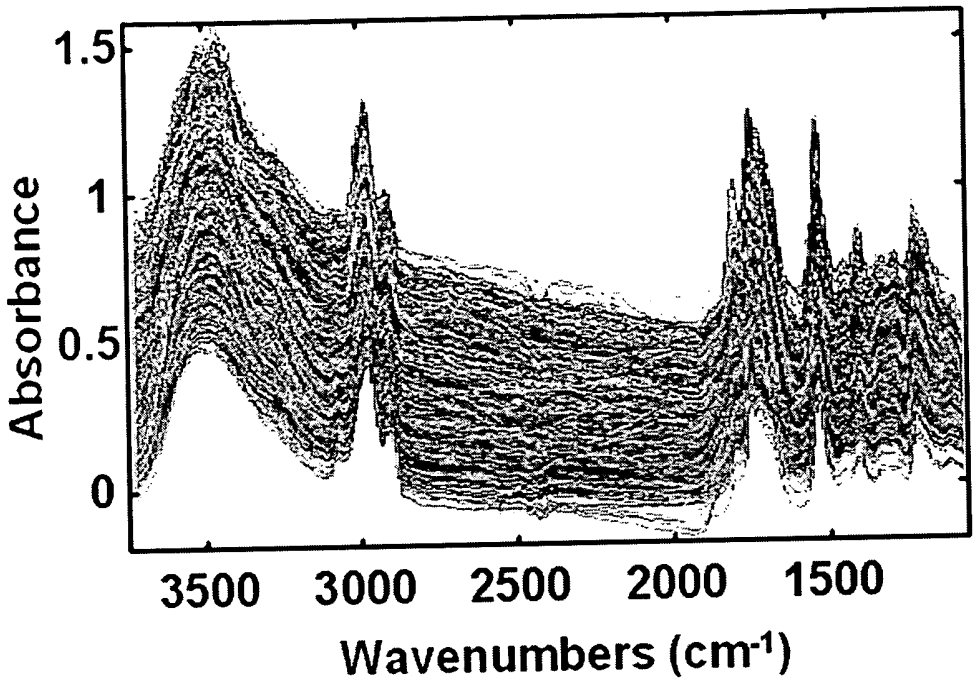



Fig. 13A

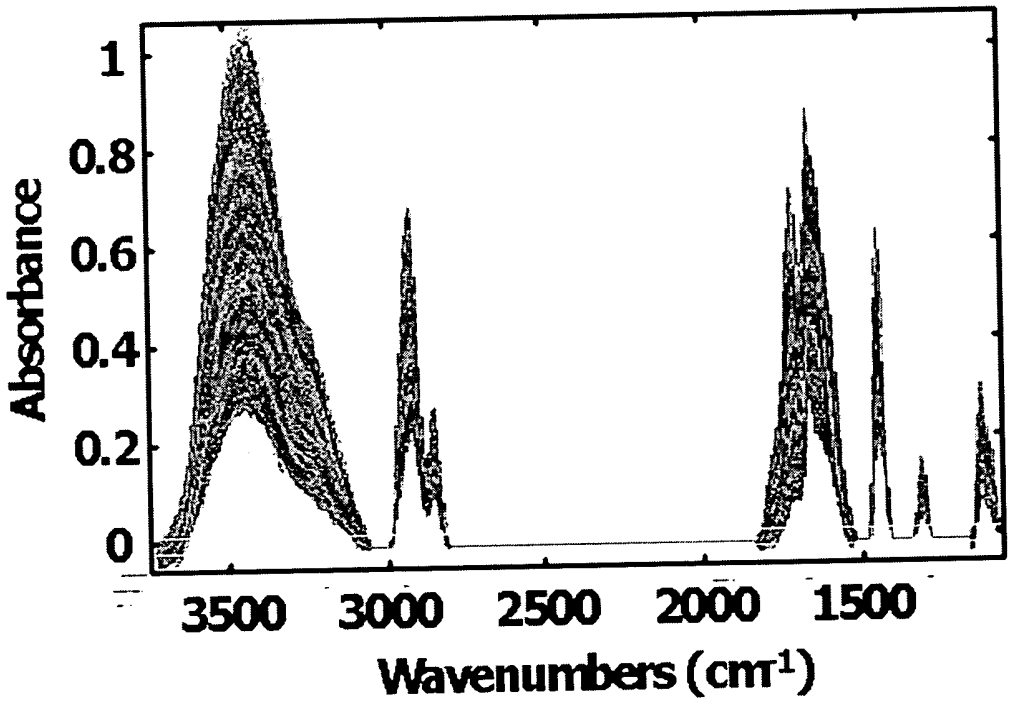



Fig. 13B

Fig. 14A

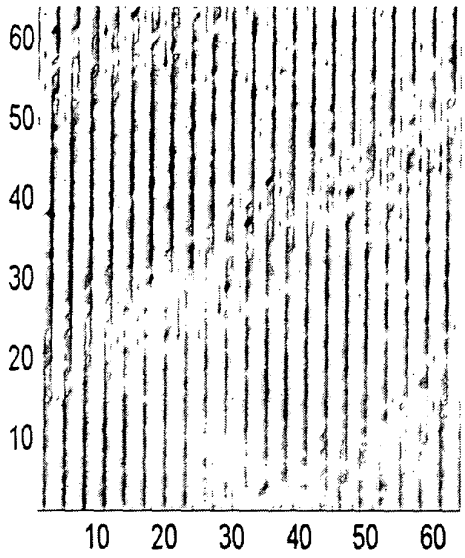



Fig. 14B

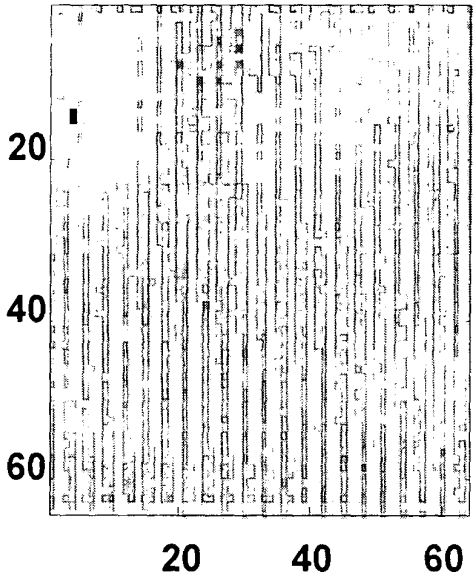
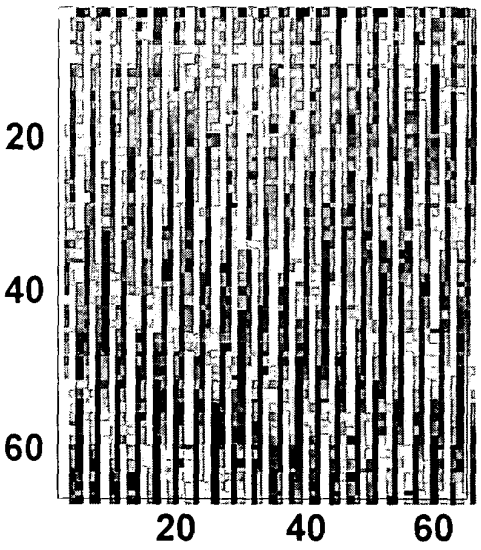



Fig. 14C



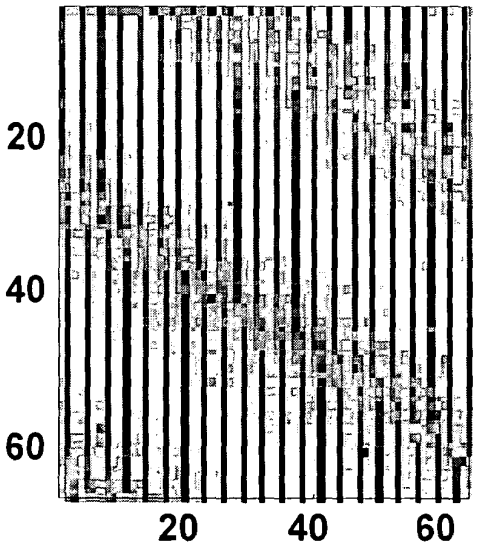


Fig. 14D